Density of states in spin-valve structure with superconducting electrodes

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Energy variation of the density of states (DOS) has been calculated in the superconductor/ferromagnet/ferromagnet/superconductor structure (SFFS) in the frame of Gorkov equations taking into account the s-d electron scattering in the ferromagnetic layers. DOS behavior is presented for the antiparallel and parallel magnetic moments alignment of two adjacent F layers. The cases of small and large values of exchange ferromagnetic field are discussed.

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I. INTRODUCTION

The possibility of the potential application of multilayers with the superconducting junctions stimulate an interest to the study of such a structures. The effect of switching between "0" and "π" states in superconductor/ferromagnet/ferromagnet/superconductor (SFFS) structures makes them useful for the microelectronic engineering. Practically it is possible to change the mutual orientation of the thin ferromagnetic layers magnetization by applying the external magnetic field. Two ferromagnetic layers separated by a nonmagnetic spacer FNF are known as "spin-valve". The combined SFFS structure with superconducting electrodes gives more interesting results. In the parallel configuration for the some ferromagnetic thickness values the Josephson current takes a zero value. At the same time for the antiparallel alignment of magnetizations the Josephson current has a non zero value. Thus, by selecting a necessary ferromagnetic layer thickness we can govern the superconducting current flow.

The presence of two ferromagnetic layers with the dirigible magnetization alignment let study two opposite cases which have their peculiarities. For the parallel magnetization alignment it is the reversion of the Josephson current sign (π state junction) that has been theoretically described [1] and experimentally observed [2, 3], and for the antiparallel case the possible current divergence.

Several authors involved in the studying of SFIFS structures (I is the insulating barier) touched upon a question of the possible enhancement of the critical Josephson current for the antiparallel magnetization alignment of the neighboring F layers under some conditions. In [4] it was found that in the case of the antiparallel orientation the critical current increases at low temperatures with increasing exchange field h and at zero temperature has a singularity when h equals to the superconducting energy gap Δ. Authors of [5] also predict the critical current enhancement for the antiparallel alignment in some interval of exchange field values. The possibility of the critical current enhancement by the exchange field in SFIFS junctions with thin F layers with antiparallel magnetization directions was discussed in the regimes os small S layer thickness [4] and bulk S electrodes [5]. Golubov et al. [6] assumed that the case of thin S layers [4] was studied in the frame of an idealized model in the tunnelling limit, which leads to a divergency of the critical current at the zero temperature, and for the bulk S case [5] an approximate method was used, so that a part of the results was obtained beyond its applicability range. Golubov et al. [6] explain the current enhancement by the singularity in density of states (DOS) which is shifted to the Fermi energy level. It happens when the effective energy shift in the ferromagnets due to the exchange field becomes equal to a local value of the effective energy gap induced into F layers. They note that in the models with DOS of the BCS type this leads to a logarithmic divergency of the critical current in the antiparallel case at zero temperature.

First of all, it should be emphasized that in most theoretical papers the SFFS structures were studied in the so-called dirty limit and for low energies, that is using the quasiclassical Usadel equations in the context of one-band model of ferromagnetic metal. Such approach does not take into account the s-d scattering of electrons which is the main scattering mechanism responsible for the kinetic properties of 3d-metals and their conductivity. Evidently, the limitation connected with the Usadel equations may be avoided by solving the full Gorkov equations which in addition take into account the s-d scattering of conducting electrons.

In the paper [7] the Josephson current in SFFS structure had been calculated in the frame of Gorkov equations taking into account the two-band model of a ferromagnet with conducting s electrons and almost localized d electrons. S layers were assumed as a simple s-wave superconductors. For the antiparallel configuration the Josephson current has no singularity at zero temperature. Consequently, from the physical point of view the results derived in [4, 5, 6] stay unclear and this question requires a more careful study. For that reason in this paper we calculate and discuss DOS for both (parallel and antiparallel) cases in the frame of Gorkov equations taking into account the s-d scattering of electrons. As it will be shown DOS does not demonstrate any divergence that makes us conclude that s-d scattering effectively de-

stroys the BCS correlation, hence, the Josephson current enhancement is suppressed.

II. GORKOV EQUATIONS

We consider the SFFS structure which consists of two semi-infinite superconducting electrodes S separated by two thin ferromagnetic layers F with the interfaces perpendicular to the z axis. Although the Green function method can be applied in more general case, for simplicity we assume the F and S materials to be equivalent on both sides of structure, and both F layers have the same thickness a which is supposed to be much smaller than the in-plane dimension of the structure. The S/F interfaces are placed at $z = \pm a$. In the mixed $(\overrightarrow{k}, z)$ representation ($\overrightarrow{k}$ is the quasi-momentum component in the XY plane of layers) the Gorkov equations for the normal $G^{ss}_{\uparrow\uparrow}$ and anomalous $F^{ss}_{\downarrow\uparrow}$ Green functions have the following form:

$$\begin{aligned}
&\left[i\omega + \frac{1}{2m}\left(\frac{\partial^2}{\partial z^2} - k^2\right) + \varepsilon_F(z) + h(z) - x_0(z)\gamma^2 G^{dd}_{\uparrow\uparrow}(z,z,\omega)\right] G^{ss}_{\uparrow\uparrow}(z,z',\omega) + \Delta(z) F^{ss}_{\downarrow\uparrow}(z,z',\omega) = \delta(z-z'),\\
&\left[i\omega - \frac{1}{2m}\left(\frac{\partial^2}{\partial z^2} - k^2\right) - \varepsilon_F(z) + h(z) - x_0(z)\gamma^2 G^{dd}_{\downarrow\downarrow}(z,z,\omega)\right] F^{ss}_{\downarrow\uparrow}(z,z',\omega) + \Delta^*(z) G^{ss}_{\uparrow\uparrow}(z,z',\omega) = 0,
\end{aligned} \tag{1}$$

where $\omega = \pi T(2n+1)$ is the Matsubara frequency at temperature T, $\varepsilon_F(z) = \varepsilon^s[\theta(-a-z) + \theta(z-a)] + \varepsilon^f\theta(z+a)\theta(a-z)$, $\varepsilon^{s(f)}$ the Fermi energy of the superconductor (ferromagnet), $\theta(z)$ the step function ($\theta(z) = 1$, if $z \geq 0$, and $\theta(z) = 0$, if $z < 0$), $\hbar = k_B = 1$. We consider that the Cooper pairing is absent in the F layer and the superconducting order parameter Δ is equal to zero in the ferromagnet, $\Delta(z) = \Delta exp(i\varphi_1)\theta(-a-z) + \Delta exp(i\varphi_2)\theta(z+a)$ ($\varphi_{1,2}$ is the order parameter phase in the left and right superconducting electrodes, correspondingly). The exchange magnetic field in the F layer: $h(z) = h\theta(z+a)\theta(-z) \pm h\theta(z)\theta(a-z)$, $h > 0$, sign $(+)$ corresponds to the parallel alignment of F layer magnetizations and $(-)$ sign should be taken for the antiparallel configuration. The s-d scattering is described in the framework of the fist Born approximation with impurity concentration $x_0(z) = x_0\theta(z+a)\theta(a-z)$ and impurity potential value γ. $G^{dd}_{\uparrow\uparrow(\downarrow\downarrow)}(z,z,\omega)$ are the diagonal Green functions of localized d electrons. Here we neglect the s-s electron scattering as it is small in comparison with the s-d scattering which are the main mechanism destroying induced superconductivity in the F layers.

In this case the Gorkov equations become linear and the solutions represent a set of plane waves with wave vectors:

$$\begin{aligned}
k_{1(2)} &= \sqrt{2m(\varepsilon^f \pm h - \frac{\kappa^2}{2m} \pm i\omega \pm \frac{i}{2\tau_{\uparrow(\downarrow)}})},\\
k_3 &= \sqrt{2m(\varepsilon^s - \frac{\kappa^2}{2m} + i\sqrt{\omega^2 + \Delta^2})},
\end{aligned} \tag{2}$$

where $k_{1(2)}$ corresponds to the majority (minority) spin electron momentum in the left F layer for the antiparallel configuration (at the same time in the right F layer with the opposite magnetization direction majority and minority momenta we label as k_4 and k_5), k_3 corresponds to the the S layer electrons. For the parallel configuration $k_1 = k_4$, $k_2 = k_5$. Here $\tau_{\uparrow(\downarrow)}$ is the spin up $(\uparrow)$ and spin down $(\downarrow)$ electron lifetime in the ferromagnet, $1/\tau_{\uparrow(\downarrow)} = -2x_0\gamma^2 ImG^{dd}_{\uparrow\uparrow(\downarrow\downarrow)}$.

The procedure of DOS calculation reduces to the diagonalization of the imaginary part of the normal Green function

$$N_{\uparrow(\downarrow)}(z) = \frac{1}{2\pi}\int \kappa d\kappa G^{ss}_{\uparrow\uparrow(\downarrow\downarrow)}(z,z,i\omega \rightarrow \omega). \tag{3}$$

Because of unhandiness of the expressions for the Green functions here we cite as an example the normal Green function only of the left F layer for spin up electrons:

$$G^{ss}_{\uparrow\uparrow}(z,z',\omega) = f_1 e^{ik_1 z} + f_2 e^{-ik_1 z}, \tag{4}$$

where f_1 and f_2 are the functions of electron momenta, ω and Δ which are given in the appendix.

In order to discuss the connection between the behavior of DOS and Josephson current which served as a motivation force of the present study we rewrite here the expression for the current derived earlier (see [7]) in the frame of Gorkov equation for the antiparallel and parallel orientation of the F-layer magnetic moments, correspondingly:

$$j_{AP}(0) = \frac{4e}{\pi}T\sum_{\omega}\int kdk\frac{(1-r^2)(1-R^2)sin\varphi}{(1-r^2)(1-R^2)cos\varphi + f_{AP}}, \tag{5}$$

$$j_P(0) = \frac{4e}{\pi}T\sum_{\omega}\int kdkRe\frac{(1-R^2)sin\varphi}{(1-R^2)cos\varphi + f_P}, \tag{6}$$

where φ is the phase difference between right and left superconducting electrodes order parameters, R and r

are reflection coefficients, f_{AP} and f_P are certain oscillatory functions which depend on the ferromagnetic layers thickness a, energy parameter ω and superconducting energy gap Δ. There is no singularity in the Josephson current for the antiparallel case at low temperatures (see Fig. 1) predicted previously in [4, 6].

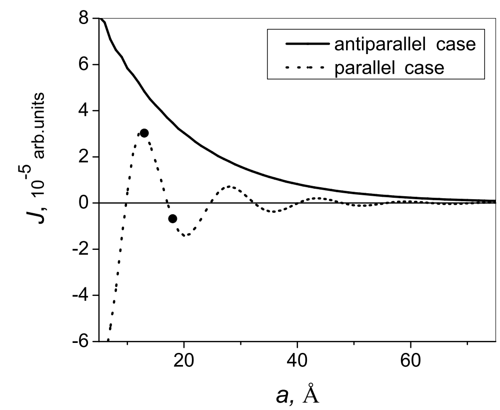

Figure 1: Josephson current J versus F layers thickness a. Fermi momenta in F layer $k^{\uparrow} = 1$ $\mathring{A}^{-1}$, $k^{\downarrow} = 0.8$ $\mathring{A}^{-1}$ ($k^{\uparrow(\downarrow)} = \sqrt{2m(\varepsilon^f \pm h})$; in S layer $k_s = 1.2$ $\mathring{A}^{-1}$. Free path of electrons in F layer $l_{\uparrow} = 100$ $\mathring{A}$ and $l_{\downarrow} = 60$ $\mathring{A}$. The critical temperature of the superconducting metal is $T_c = 4$ K.

III. ANTIPARALLEL CASE

Antiparallel case. In Ref.[6] the authors derive the expression for DOS which demonstrate the energy renormalization due to exchange field in SFIFS (I - insulating barier). For a certain exchange field value h DOS expression yields the singularity which is shifted to the Fermi level that leads to the logarithmic divergency of the critical current at low temperatures. However, the authors avoid the singularity problem by taking the low barrier transparency which makes peaks broader and in such a way suppresses the singularity.

In Ref.[8] energy variation of DOS was investigated in the S/F structure. This case resembles more to the SFFS structure with parallel magnetizations of F layers, but here we can note that just as in Ref.[6] DOS has a peak and a region of zero value within the energy gap in much the same way as in S/N structures (N is the normal metal)[9].

Both calculations were made for the small value of the exchange field $h \sim \Delta$. Our computation for the same range of exchange field is depicted in Fig. 2. As one can see the DOS has a BCS behavior outside the energy gap and usual divergence at $\omega = \Delta$. However there in no any singularities or peaks within the energy gap and DOS never equals to zero. Last peculiarity may be explained by the destructive role of s-d electron scattering in F layers which destroys the Cooper pairs. The curves a,b,c were plotted for the different values of the free path $l_{\uparrow(\downarrow)}$ of spin up(down) electrons in the F layer, $l_{\uparrow(\downarrow)} = v_F \tau_{\uparrow(\downarrow)}$, v_F is the Fermi velocity in the F layer. For the small values of free path (i.e. in the case of the strong s-d scattering) the hollow becomes smaller and DOS approaches the constant as in the bulk ferromagnet. The inset of Fig. 2 depicts energy DOS variation within the energy gap for the different F layers thickness a. For the decreasing values of a DOS becomes more close to zero as in a bulk superconductor. The peaks in DOS appear for the large

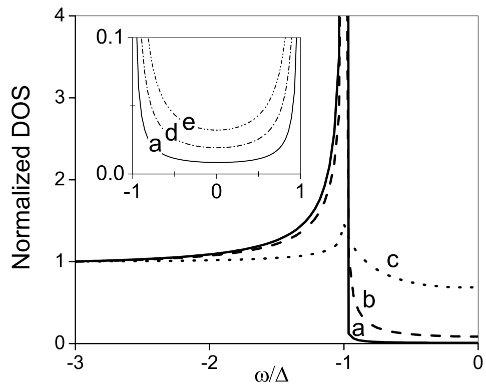

Figure 2: Energy variation of DOS at the left F/S border ($z = -a$) for the antiparallel case for the small value of exchange energy $h \sim \Delta$, $\Delta = 1.4\, 10^{-3} eV$. a) $a = 7$ $\mathring{A}$, $l^{\uparrow} = 500$ $\mathring{A}$; b) $a = 7$ $\mathring{A}$, $l_{\uparrow} = 100$ $\mathring{A}$; c) $a = 7$ $\mathring{A}$, $l_{\uparrow} = 10$ $\mathring{A}$; d) $a = 15$ $\mathring{A}$, $l_{\uparrow} = 500$ $\mathring{A}$; e) $a = 25$ $\mathring{A}$, $l_{\uparrow} = 500$ $\mathring{A}$.

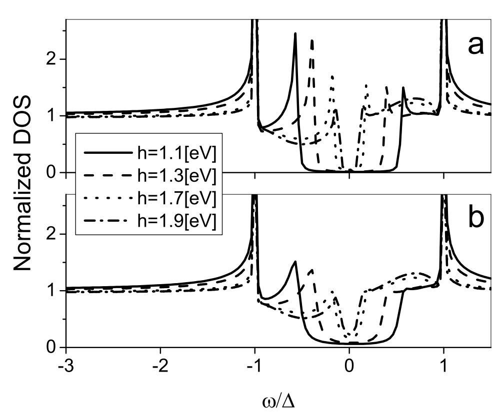

Figure 3: Energy variation of DOS at the F/S border ($z = a$) for the antiparallel alignment of F-layers magnetization. Fermi momentum of electrons in S-layer: $k_s = 1$ $\mathring{A}^{-1}$. In the F-layer for the electrons with spin up: $k^{\uparrow} = 1$ $\mathring{A}^{-1}$, $k^{\uparrow(\downarrow)} = \sqrt{2m(\varepsilon^f \pm h)}$. a) $l_{\uparrow} = 500$ $\mathring{A}$; b) $l_{\uparrow} = 100$ $\mathring{A}$.

values of the ferromagnetic exchange field $h \sim 10^3 \Delta$ (the

case of a strong ferromagnet). Outside the energy gap DOS stays of a BCS type and within the gap DOS has two symmetrical peaks (Fig. 3a). As in Ref. [6] they can be shifted closer to the Fermi energy ($\omega = 0$) but at the same time their size diminishes and there is no any singularity at the very zero. For the smaller values of free path and large values of s-d scattering parameter (Fig. 3b) the peaks lose their pointed shape.

In both cases of small and large values of ferromagnetic exchange field DOS does not demonstrate any divergence at the Fermi level which is in a good agreement with the calculated earlier Josephson current dependencies for the antiparallel alignment of F layers magnetic moments.

IV. PARALLEL CASE

For the small values of the exchange field $h \sim \Delta$ in the parallel case there are no any significant changes in DOS in comparison with the antiparallel case presented in Fig. 2. But for the large values of h in contrast to the antiparallel case multiple electron reflection takes place that graphically manifests itself in multiple resonance peaks in DOS within the energy gap (see Fig. 4).

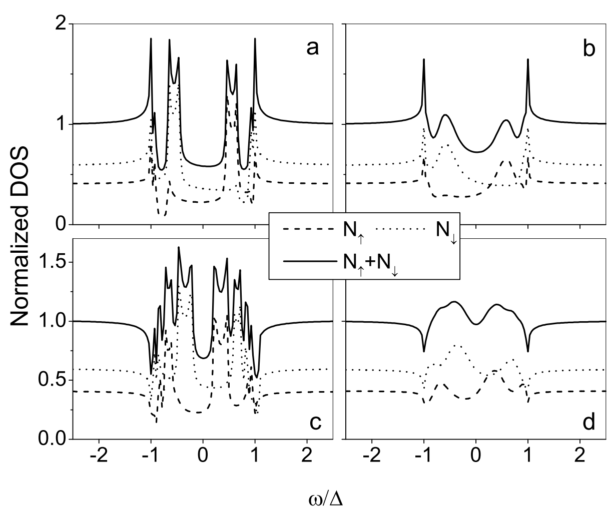

Figure 4: Energy variation of DOS at $z = 0$ for the parallel alignment of F-layers magnetization. Fermi momentum of electrons in S-layer: $k_s = 1$ Å^{-1}. In the F-layer for the electrons with spin up: $k^{\uparrow} = 1$ Å^{-1} and exchange field $h \sim 10^3\Delta$. a) "0" state: $a = 14$ Å, $l_{\uparrow} = 500$ Å; b) "0" state: $a = 14$ Å, $l_{\uparrow} = 100$ Å; c) "π" state: $a = 19$ Å, $l_{\uparrow} = 500$ Å; d) "π" state: $a = 19$ Å, $l^{\uparrow} = 100$ Å. Dashed line: DOS for spin up $N_{\uparrow}$. Dotted line: DOS for spin down $N_{\downarrow}$. Solid line: $N_{\uparrow} + N_{\downarrow}$.

This fact may be explained in the following way. The antiparallel alignment is more favorable for the relatively free diffusion of the Cooper pair electrons which have the opposite spin direction. Possible destruction of the pair in the first F layer compensates by the presence of the second F layer with the opposite magnetic moment alignment and reversed majority and minority spins. While in the parallel case for the large values of the exchange field $h \gg \Delta$, when spin up and spin down electron energies differ notably, only one electron in the pair whose Fermi energy is the same in the F and S layers may travel relatively free. Hence, the initial pair destroys rapidly and the multiple reflections becomes possible as it happens in the potential well.

DOS dependencies in Fig. 4 are plotted for the different values of free path. For increasing value of s-d scattering in the F layers multiple irregularities are smoothed over and energy DOS variations resemble to those calculated near the S/F border of bilayer in [10] in the frame of Gorkov equations. So called "0" and "π" states are presented in Ref. [2]. Due to the oscillations of the superconducting order parameter induced in the F layers in the "π" state the DOS shape is reversed with the respect to the normal "0" state. Instead of usual BCS energy dependence with two peaks at $\omega = \pm\Delta$ DOS has two dips at these energies values. As at was discussed earlier the Josephson current varies its sign in the parallel case [5, 6, 7], (+) corresponds to the "0" phase and (−) to the "π" phase. We have compared DOS behavior with presented in Fig. 1 Josephson current oscillation from "0" to "π" state in the parallel case. Thick points in Fig. 1 correspond to the F layers thicknesses a which had been chosen for that comparison. Indeed, for these values of a DOS demonstrates the same transition between "0" and "π" states (Fig. 4 a,b and Fig. 4 c,d, correspondingly).

V. SUMMARY

In this paper the energy DOS variation had been studied in the SFFS structure for the antiparallel and parallel magnetic moments alignment of two adjacent F layers. It was shown that there in no any singularity in DOS in the antiparallel case that is in a good agreement with calculated earlier Josephson current behavior in the same model. In the parallel case the presence of "0" and "π" states had been shown.

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APPENDIX: EXPRESSIONS FOR THE COEFFICIENTS IN EQ. (4)

$$f_{1,2}=\frac{e^{-iak_4}}{4k_1k_4}(k_1\pm k_4)\left(A_1(k_3+k_4)+A_2(k_4-k_3^*)\right)+\frac{e^{iak_4}}{4k_1k_4}(k_1\mp k_4)\left(A_1(k_4-k_3)+A_2(k_4+k_3^*)\right),$$

$$\begin{aligned}A_{1,2} &= \tfrac{1}{den}\left[\pm(B_2k_1-B_1k_3^*)(k_3t_{2,1}+k_2t_{4,3})\pm\Delta_2(B_1k_3+B_2k_1)(k_2t_{4,3}-k_3^*t_{2,1})\pm\right.\\ &\qquad\left.\pm\Delta_1\Delta_2k_1(k_3+k_3^*)(B_2c_{2,1}-B_1c_{4,3})\right],\end{aligned}$$

$$\begin{aligned}den &= k_2(k_3+k_3^*)(t_2t_3-t_1t_4)+\Delta_1\Delta_2k_1(k_3+k_3^*)(c_1c_4+c_2c_3)+\\ &+\Delta_1\left((k_1c_4-k_3^*c_2)(k_3t_1+k_2t_3)+(k_3^*c_1-k_1c_3)(k_3t_2+k_2t_4)\right)+\\ &+\Delta_2\left((k_1c_4+k_3c_2)(k_2t_3-k_3^*t_1)+(k_3c_1-k_1c_3)(k_3^*t_2-k_2t_4)\right),\end{aligned}$$

$$B_{1,2}=i(e^{-iz'k_1}e^{-iak_1}\mp e^{iz'k_1}e^{iak_1})/2k_1,\ \ \Delta_{1,2}=ie^{-i\varphi_1}\tfrac{\sqrt{\omega^2+\Delta^2}\pm i\omega}{\Delta},$$

$$\begin{aligned}c_{1,3} &= \tfrac{e^{-iak_1}}{4k_1k_4}\left[e^{-iak_4}(k_3+k_4)(k_1+k_4)+e^{iak_4}(k_4-k_3)(k_1-k_4)\right]\pm\\ &\pm\tfrac{e^{iak_1}}{4k_1k_4}\left[e^{-iak_4}(k_3+k_4)(k_1-k_4)+e^{iak_4}(k_4-k_3)(k_1+k_4)\right],\\ c_{2,4} &= \tfrac{e^{-iak_1}}{4k_1k_4}\left[e^{-iak_4}(k_4-k_3^*)(k_1+k_4)+e^{iak_4}(k_4+k_3^*)(k_1-k_4)\right]\pm\\ &\pm\tfrac{e^{iak_1}}{4k_1k_4}\left[e^{-iak_4}(k_4-k_3^*)(k_1-k_4)+e^{iak_4}(k_4+k_3^*)(k_1+k_4)\right],\end{aligned}$$

$$\begin{aligned}t_{1,3} &= \Delta_1\tfrac{e^{iak_5}}{4k_2k_5}\left[e^{iak_2}(k_2-k_3)(k_2+k_5)+e^{-iak_2}(k_2+k_3)(k_5-k_2)\right]\pm\\ &\pm\Delta_1\tfrac{e^{-iak_5}}{4k_2k_5}\left[e^{iak_2}(k_2-k_3)(k_5-k_2)+e^{-iak_2}(k_2+k_3)(k_2+k_5)\right],\\ t_{2,4} &= -\Delta_2\tfrac{e^{iak_5}}{4k_2k_5}\left[e^{iak_2}(k_2+k_3^*)(k_2+k_5)+e^{-iak_2}(k_2-k_3^*)(k_5-k_2)\right]\mp\\ &\mp\Delta_2\tfrac{e^{-iak_5}}{4k_2k_5}\left[e^{iak_2}(k_2+k_3^*)(k_5-k_2)+e^{-iak_4}(k_2-k_3^*)(k_2+k_5)\right].\end{aligned}$$

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